wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 12:35 AM EDT

PDB ID	:	4H0L
Title	:	Cytochrome b6f Complex Crystal Structure from Mastigocladus laminosus with n-Side Inhibitor NQNO
Authors	:	Hasan, S.S.; Yamashita, E.; Baniulis, D.; Cramer, W.A.
Deposited on	:	2012-09-08
Resolution	:	3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

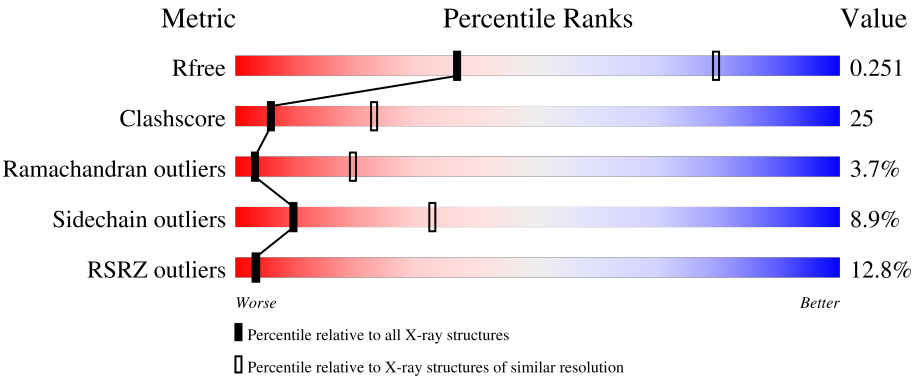
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	68% 28%
2	B	160	54% 41%
3	C	289	18% 51% 40% 7%
4	D	179	37% 50% 33% 6% 10%
5	E	32	9% 25% 53% 22%

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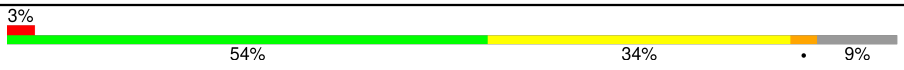
Mol	Chain	Length	Quality of chain
6	F	35	
7	G	37	
8	H	29	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	UMQ	A	306	X	-	-	X
12	UMQ	A	307	X	-	-	-
12	UMQ	A	309	X	-	-	-
12	UMQ	C	301	X	-	-	X
13	QNO	A	308	X	-	-	-
14	CLA	B	202	X	-	-	-
16	SQD	D	201	X	-	-	X
17	BCR	G	101	-	X	-	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 16219 atoms, of which 8226 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	H	N	O	S	0	0	0
			3420	1132	1722	270	286	10			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	160	Total	C	H	N	O	S	0	0	0
			2558	841	1309	193	209	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	286	Total	C	H	N	O	S	0	0	0
			4419	1406	2219	366	421	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	PRO	GLU	SEE REMARK 999	UNP P83793

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	161	Total	C	H	N	O	S	0	0	0
			2460	791	1224	213	225	7			

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	32	Total	C	H	N	O	S	0	0	0
			532	179	284	34	34	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	32	502	165	260	35	40	2	0	0	0

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
7	G	37	572	188	289	44	50	1	0	0	0

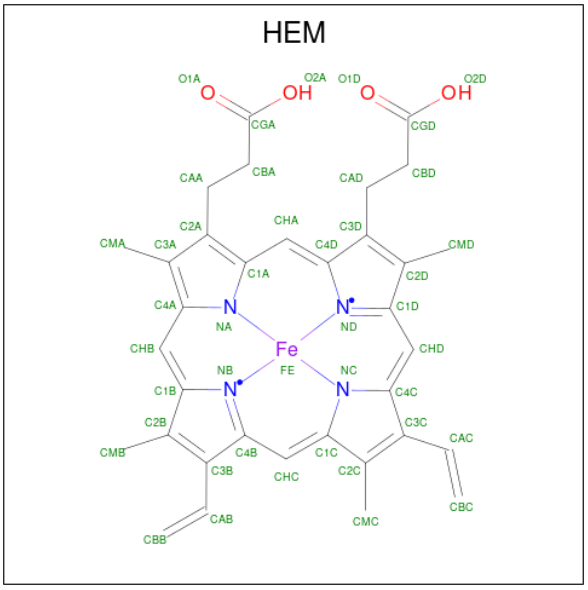
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
8	H	29	469	156	239	36	36	2	0	0	0

- Molecule 9 is CADMIUM ION (three-letter code: CD) (formula: Cd).

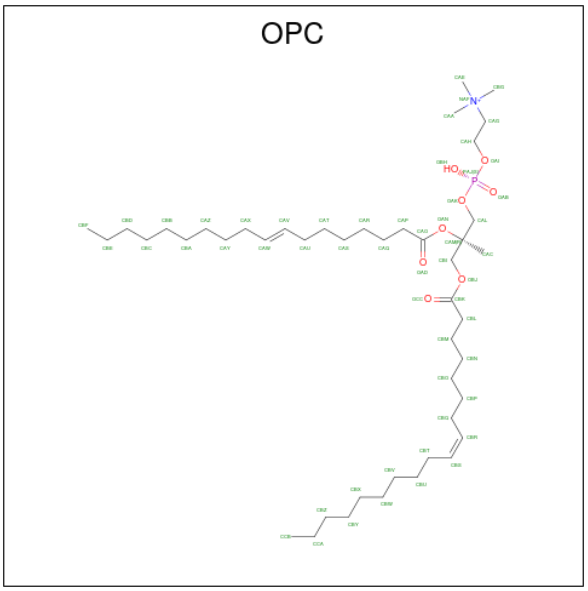
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
9	A	1	1	1	0	0
9	B	1	Total	Cd	0	0
			1	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



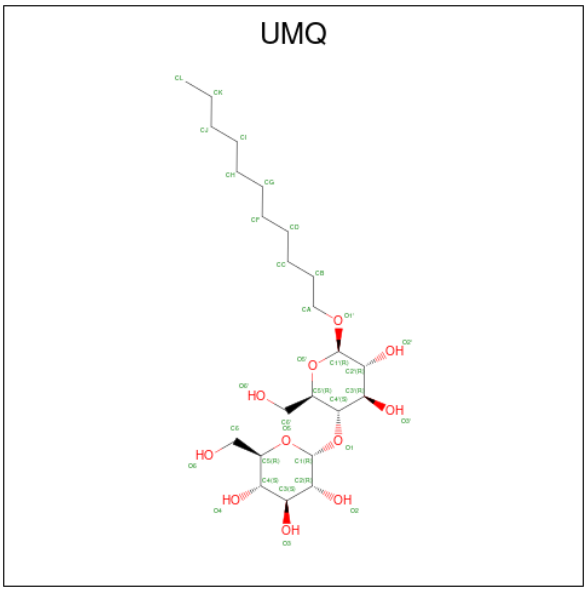
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 11 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: $C_{45}H_{87}NO_8P$).



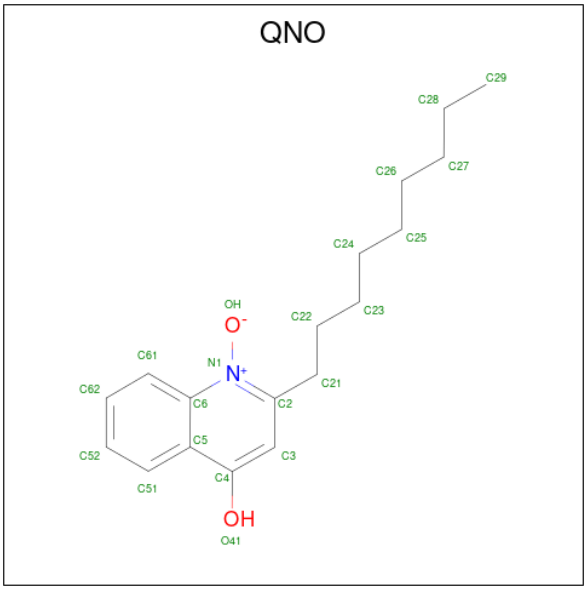
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	A	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		
11	B	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



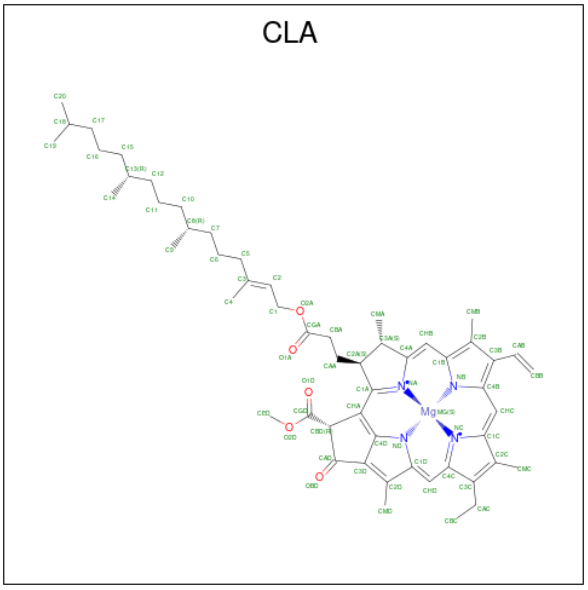
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	C	1	Total	C	H	O	0	0
			78	23	44	11		

- Molecule 13 is 2-NONYL-4-HYDROXYQUINOLINE N-OXIDE (three-letter code: QNO) (formula: $C_{18}H_{25}NO_2$).



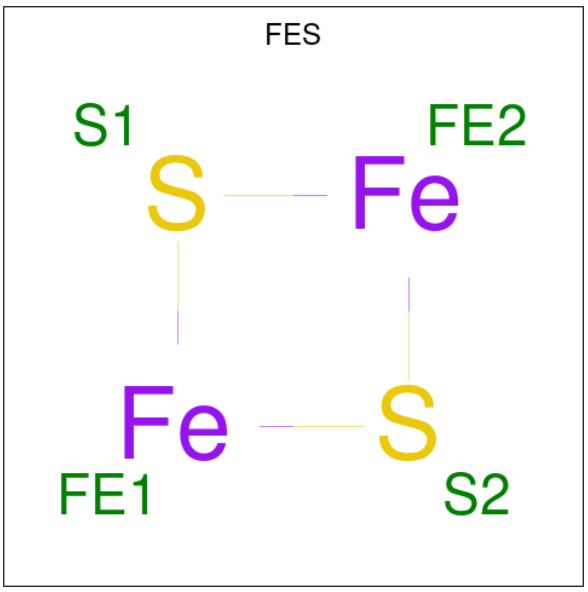
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	N	O	0	0
			46	18	25	1	2		

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



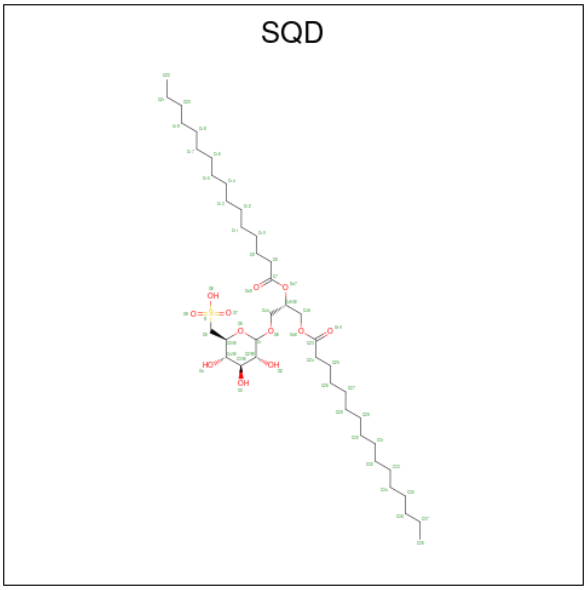
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			127	55	62	1	4	5		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



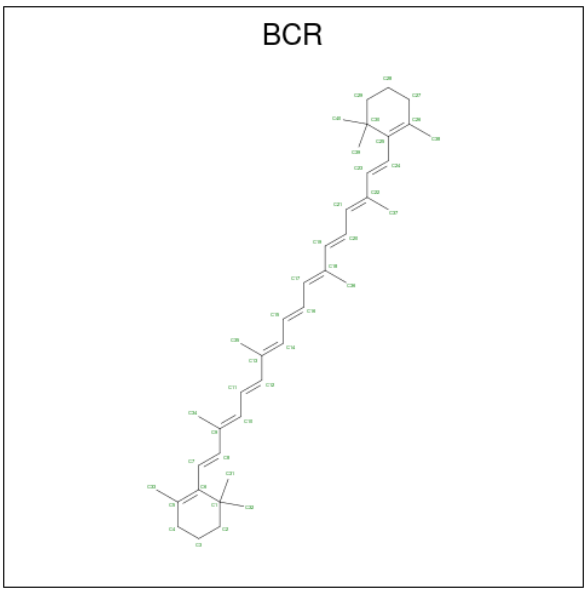
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	1	Total Fe S 4 2 2	0	0

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	D	1	Total C H O S 131 41 78 11 1	1	0

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total C H 96 40 56	0	0

- Molecule 18 is water.

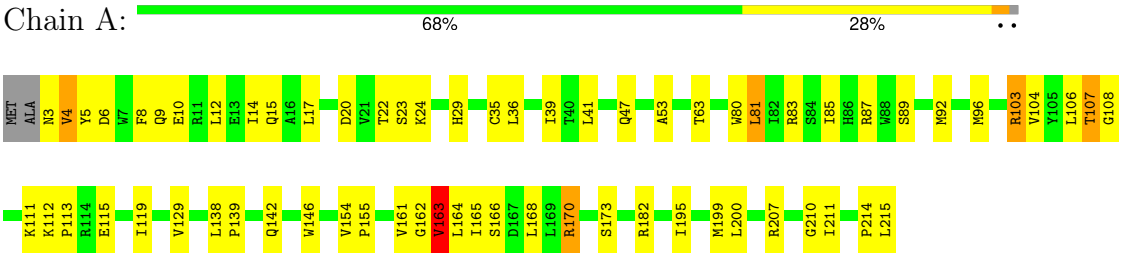
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	2	Total O 2 2	0	0
18	B	3	Total O 3 3	0	0
18	C	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

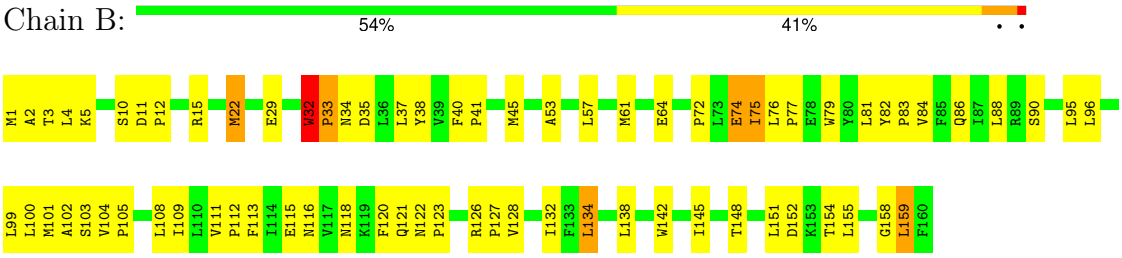
• Molecule 1: Cytochrome b6

Chain A:



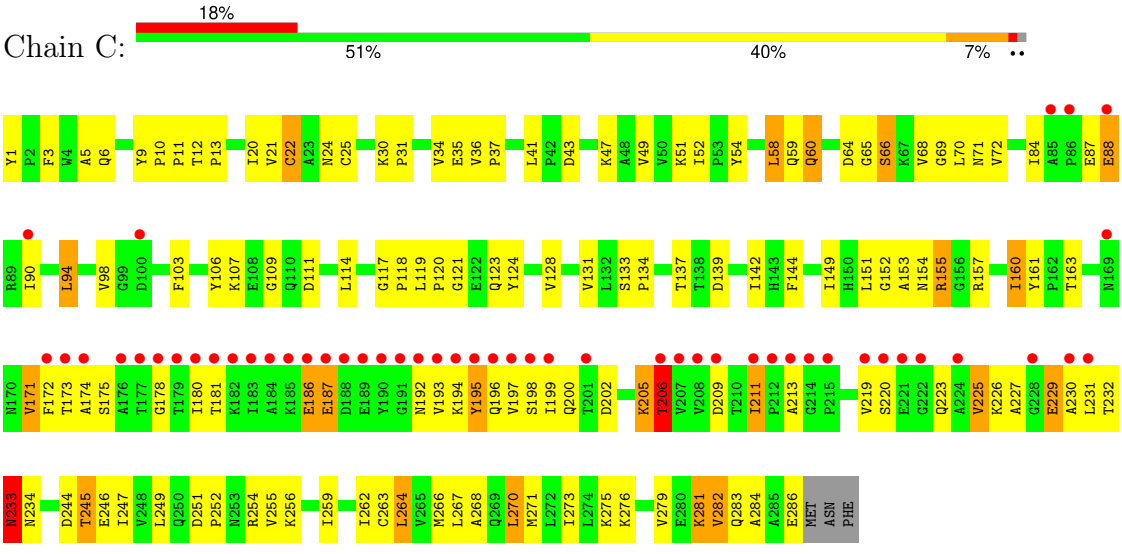
• Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:



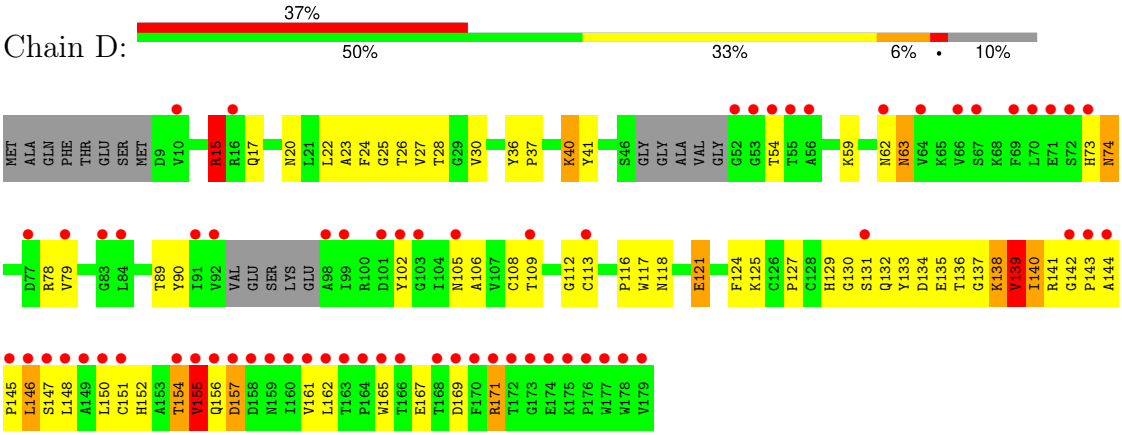
• Molecule 3: Apocytochrome f

Chain C:



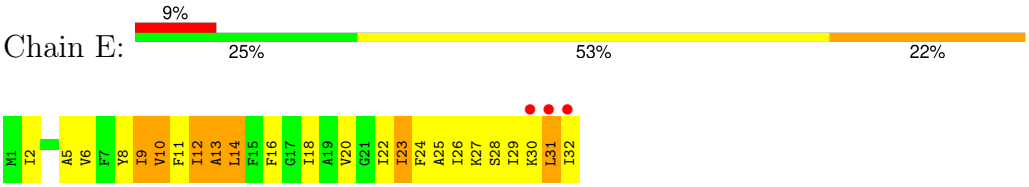
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit

Chain D:



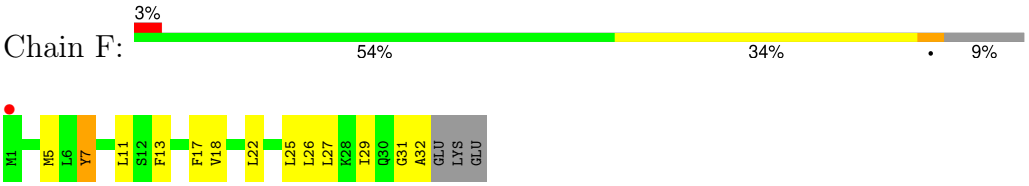
• Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:



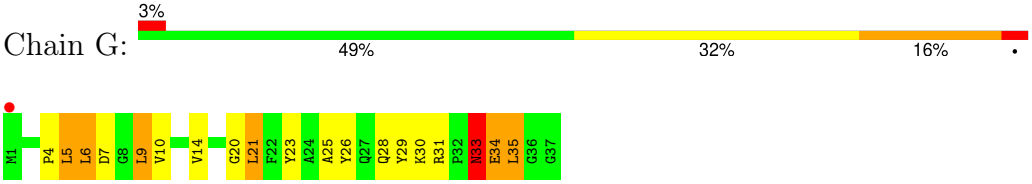
• Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:



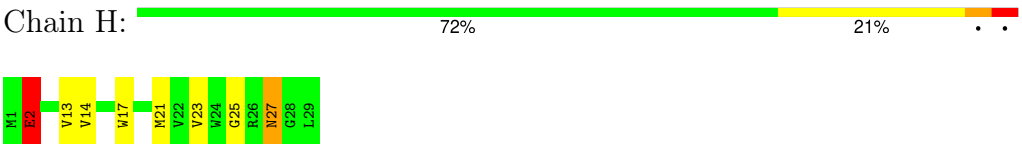
• Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:



• Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	159.13Å 159.13Å 362.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.25 48.45 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.45-3.25) 99.6 (48.45-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0029, PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.218 , 0.247 0.225 , 0.251	Depositor DCC
R_{free} test set	2186 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	96.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 86.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16219	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CLA, CD, HEM, QNO, UMQ, SQD, OPC, BCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/1750	0.55	0/2388
2	B	0.34	0/1288	0.63	1/1765 (0.1%)
3	C	0.37	0/2248	0.60	0/3061
4	D	0.29	0/1267	0.58	1/1725 (0.1%)
5	E	0.47	0/253	0.94	0/340
6	F	0.40	0/246	0.52	0/331
7	G	0.42	0/289	0.75	1/391 (0.3%)
8	H	0.40	0/236	0.55	0/323
All	All	0.37	0/7577	0.61	3/10324 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
5	E	0	1
7	G	0	1
8	H	0	2
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	32	TRP	C-N-CD	-8.06	102.87	120.60
7	G	35	LEU	CA-CB-CG	5.34	127.58	115.30
4	D	15	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	2	ALA	Peptide
2	B	32	TRP	Peptide
5	E	28	SER	Peptide
7	G	33	ASN	Peptide
8	H	2	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1698	1722	1720	64	2
2	B	1249	1309	1308	59	0
3	C	2200	2219	2218	119	2
4	D	1236	1224	1219	92	0
5	E	248	284	284	47	0
6	F	242	260	260	15	0
7	G	283	289	289	25	0
8	H	230	239	239	10	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	129	90	90	13	0
10	C	43	30	30	11	0
11	A	54	83	83	9	0
11	B	54	83	83	4	0
12	A	102	129	128	8	0
12	C	34	44	42	4	0
13	A	21	25	25	2	0
14	B	65	62	71	5	0
15	D	4	0	0	1	0
16	D	53	78	74	18	0
17	G	40	56	56	9	0
18	A	2	0	0	0	0
18	B	3	0	0	0	0
18	C	1	0	0	0	0
All	All	7993	8226	8219	406	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 406 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:ARG:NH1	5:E:30:LYS:O	1.87	1.07
3:C:22:CYS:SG	10:C:302:HEM:C3B	2.51	1.04
3:C:271:MET:HE1	4:D:22:LEU:HD23	1.44	0.99
3:C:25:CYS:SG	10:C:302:HEM:CAC	2.51	0.99
4:D:25:GLY:HA3	16:D:201:SQD:H341	1.42	0.99

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:NZ	3:C:87:GLU:OE1[8_665]	1.82	0.38
1:A:112:LYS:HZ2	3:C:87:GLU:OE1[8_665]	1.41	0.19

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	211/215 (98%)	187 (89%)	19 (9%)	5 (2%)	6 28
2	B	158/160 (99%)	143 (90%)	11 (7%)	4 (2%)	5 28
3	C	284/289 (98%)	235 (83%)	41 (14%)	8 (3%)	5 25
4	D	155/179 (87%)	123 (79%)	22 (14%)	10 (6%)	1 9
5	E	30/32 (94%)	16 (53%)	11 (37%)	3 (10%)	0 3
6	F	30/35 (86%)	29 (97%)	1 (3%)	0	100 100
7	G	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1 5
8	H	27/29 (93%)	26 (96%)	0	1 (4%)	3 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	930/976 (95%)	785 (84%)	111 (12%)	34 (4%)	3 19

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
2	B	33	PRO
2	B	34	ASN
2	B	75	ILE
3	C	66	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	183/184 (100%)	172 (94%)	11 (6%)	19 49
2	B	137/137 (100%)	127 (93%)	10 (7%)	14 40
3	C	240/243 (99%)	212 (88%)	28 (12%)	5 21
4	D	133/146 (91%)	122 (92%)	11 (8%)	11 36
5	E	25/25 (100%)	20 (80%)	5 (20%)	1 5
6	F	24/27 (89%)	22 (92%)	2 (8%)	11 36
7	G	28/28 (100%)	25 (89%)	3 (11%)	6 25
8	H	24/24 (100%)	23 (96%)	1 (4%)	30 59
All	All	794/814 (98%)	723 (91%)	71 (9%)	9 32

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	150	LEU
4	D	155	VAL
6	F	5	MET
3	C	88	GLU
3	C	60	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
3	C	154	ASN
3	C	233	ASN
4	D	63	ASN
4	D	159	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	OPC	B	203	-	53,53,54	1.06	3 (5%)	59,61,64	0.95	3 (5%)
12	UMQ	A	306	-	35,35,35	1.16	5 (14%)	46,46,46	1.80	8 (17%)
17	BCR	G	101	-	41,41,41	2.20	20 (48%)	56,56,56	2.44	26 (46%)
10	HEM	A	303	1	42,50,50	1.91	5 (11%)	46,82,82	1.57	7 (15%)
16	SQD	D	201	-	51,53,54	3.21	17 (33%)	60,63,65	2.46	18 (30%)
13	QNO	A	308	10	21,22,22	2.76	5 (23%)	22,28,28	2.65	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	OPC	A	305	-	53,53,54	1.02	4 (7%)	59,61,64	1.14	4 (6%)
10	HEM	C	302	3	42,50,50	1.91	6 (14%)	46,82,82	1.79	13 (28%)
10	HEM	A	302	1	42,50,50	1.87	6 (14%)	46,82,82	1.56	7 (15%)
12	UMQ	A	307	-	35,35,35	1.26	5 (14%)	46,46,46	2.04	13 (28%)
12	UMQ	A	309	-	35,35,35	1.23	5 (14%)	46,46,46	2.63	18 (39%)
14	CLA	B	202	18	63,73,73	1.38	6 (9%)	74,113,113	1.55	12 (16%)
15	FES	D	200	4	0,4,4	-	-	-		
10	HEM	A	304	13,18	42,50,50	2.12	7 (16%)	46,82,82	1.63	6 (13%)
12	UMQ	C	301	-	35,35,35	1.29	5 (14%)	46,46,46	2.00	10 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OPC	B	203	-	-	23/57/57/60	-
12	UMQ	A	306	-	1/1/10/10	10/20/60/60	0/2/2/2
17	BCR	G	101	-	-	24/29/63/63	0/2/2/2
10	HEM	A	303	1	-	3/12/54/54	-
16	SQD	D	201	-	3/3/9/9	27/49/65/69	0/1/1/1
13	QNO	A	308	10	1/1/0/0	4/9/9/9	0/2/2/2
11	OPC	A	305	-	-	24/57/57/60	-
12	UMQ	A	307	-	2/2/10/10	8/20/60/60	0/2/2/2
12	UMQ	A	309	-	4/4/10/10	16/20/60/60	0/2/2/2
10	HEM	A	302	1	-	4/12/54/54	-
10	HEM	C	302	3	-	3/12/54/54	-
14	CLA	B	202	18	2/2/17/20	15/37/115/115	-
15	FES	D	200	4	-	-	0/1/1/1
10	HEM	A	304	13,18	-	6/12/54/54	-
12	UMQ	C	301	-	1/1/10/10	7/20/60/60	0/2/2/2

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	C2-C3	-10.49	1.32	1.52
16	D	201	SQD	O6-C44	9.55	1.60	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	304	HEM	C3D-C2D	8.23	1.54	1.36
16	D	201	SQD	C8-C7	7.78	1.73	1.50
10	C	302	HEM	C3D-C2D	7.68	1.53	1.36

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	201	SQD	C3-C4-C5	9.62	119.63	109.99
13	A	308	QNO	C3-C2-N1	-9.08	108.97	118.94
13	A	308	QNO	C4-C3-C2	-7.35	112.89	118.45
14	B	202	CLA	C4A-NA-C1A	6.94	109.85	106.68
12	A	309	UMQ	O5'-C1'-C2'	6.56	123.84	110.37

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	306	UMQ	C4'
12	A	307	UMQ	C2
12	A	307	UMQ	C2'
12	A	309	UMQ	C2
12	A	309	UMQ	C3'

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	305	OPC	CAH-OAI-PAJ-OAB
11	A	305	OPC	NAF-CAG-CAH-OAI
11	B	203	OPC	CAH-OAI-PAJ-OAK
11	B	203	OPC	CAH-OAI-PAJ-OAB
11	B	203	OPC	NAF-CAG-CAH-OAI

There are no ring outliers.

15 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	203	OPC	4	0
12	A	306	UMQ	5	0
17	G	101	BCR	9	0
10	A	303	HEM	1	0
16	D	201	SQD	18	0
13	A	308	QNO	2	0

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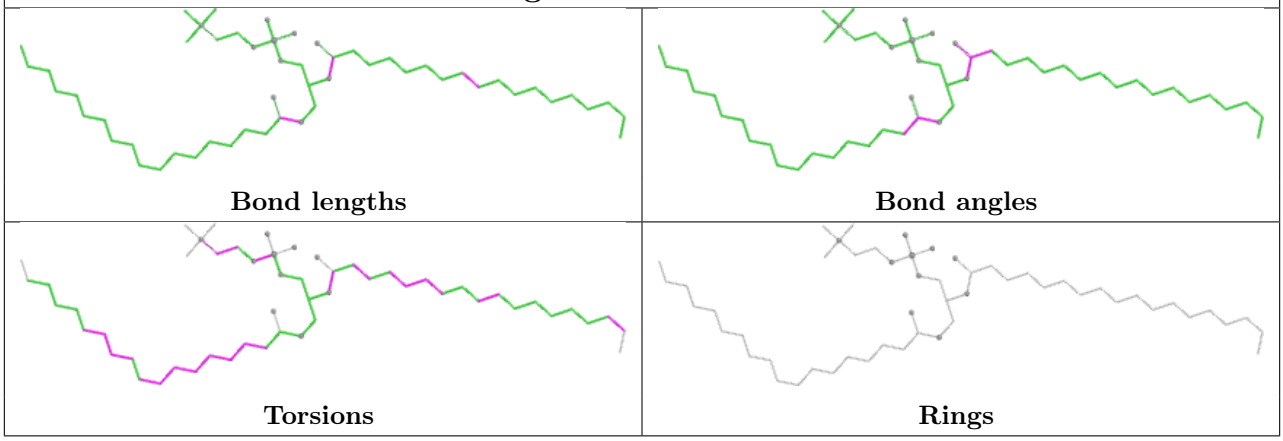
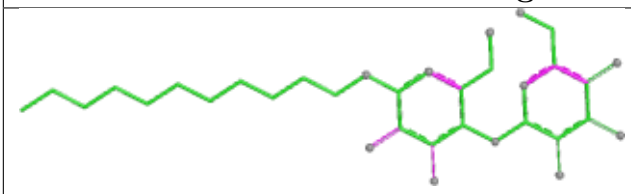
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	305	OPC	9	0
10	C	302	HEM	11	0
10	A	302	HEM	2	0
12	A	307	UMQ	1	0
12	A	309	UMQ	2	0
14	B	202	CLA	5	0
15	D	200	FES	1	0
10	A	304	HEM	10	0
12	C	301	UMQ	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

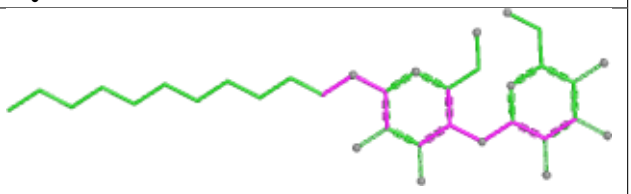
Ligand OPC B 203



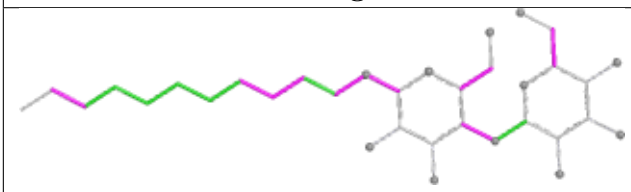
Ligand UMQ A 306



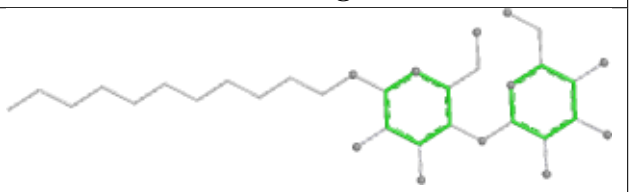
Bond lengths



Bond angles

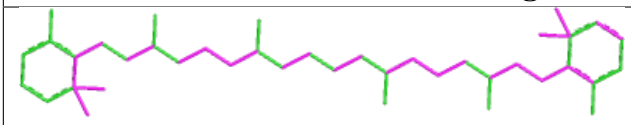


Torsions



Rings

Ligand BCR G 101



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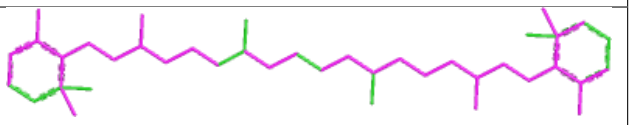

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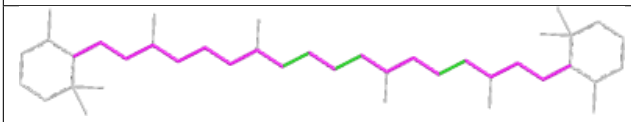

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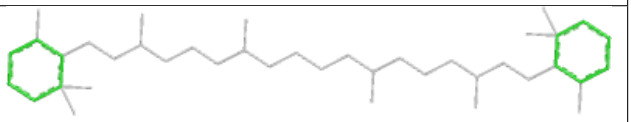
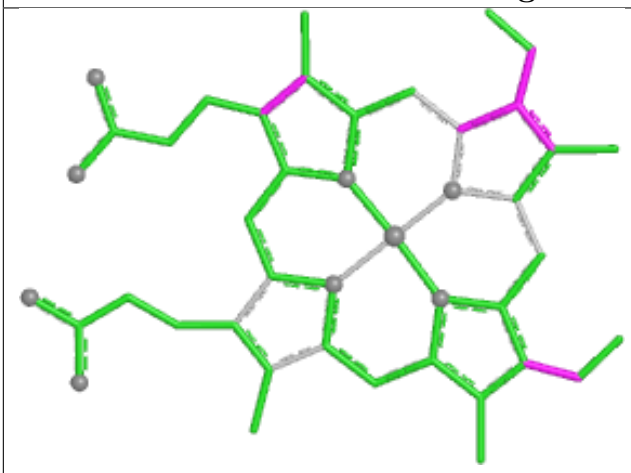


Rings

Ligand HEM A 303



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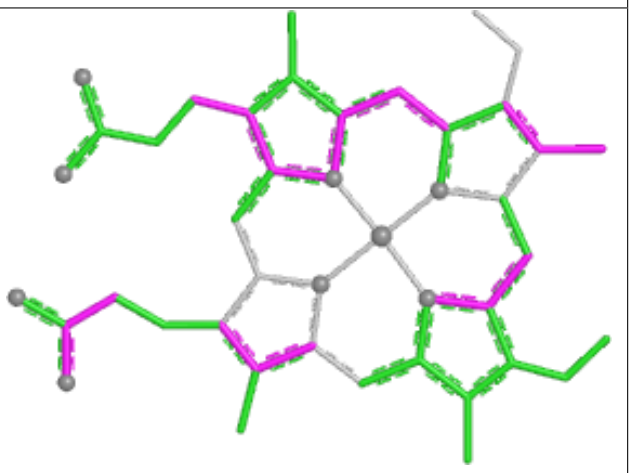
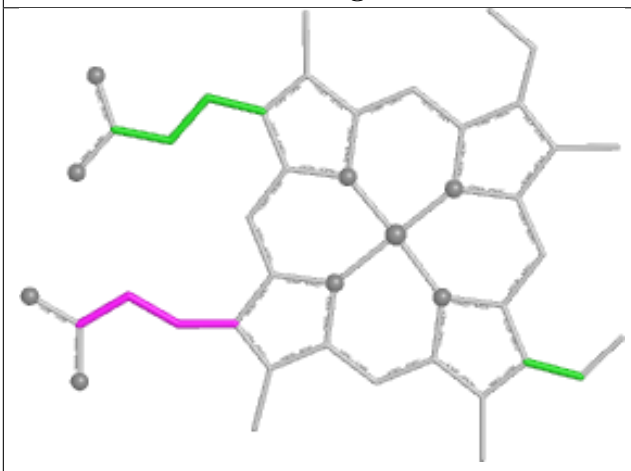
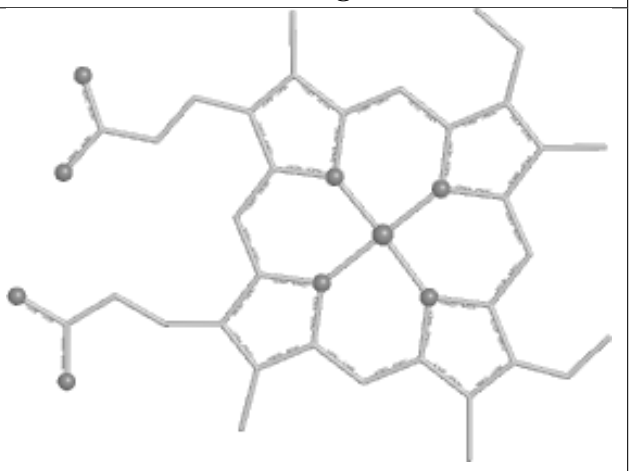


Bond angles

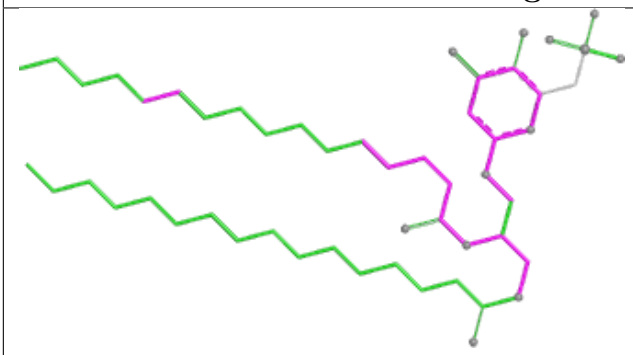


Torsions



Rings

Ligand SQD D 201



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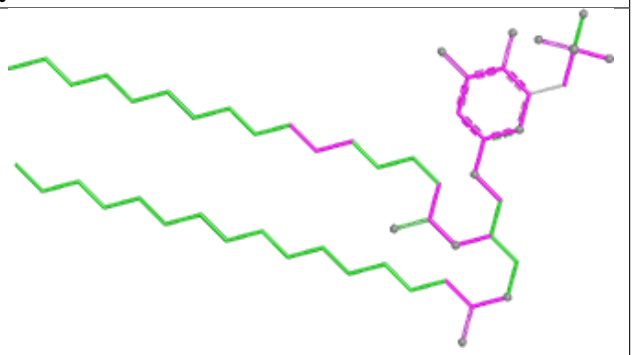
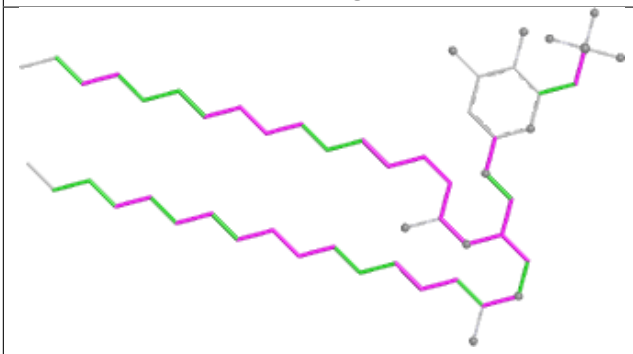
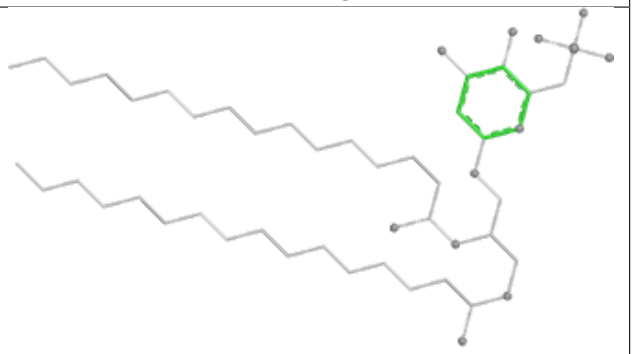


Bond angles

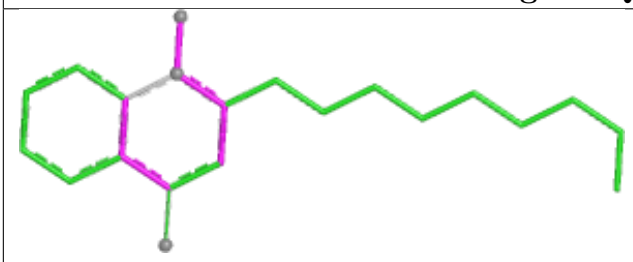


Torsions

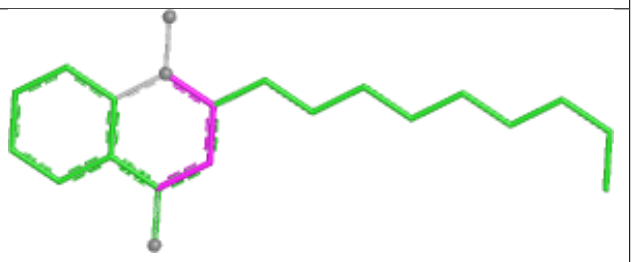


Rings

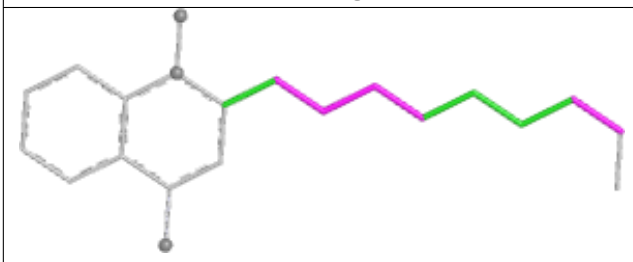
Ligand QNO A 308



Bond lengths



Bond angles



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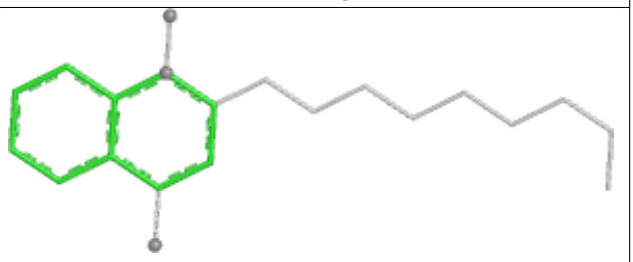
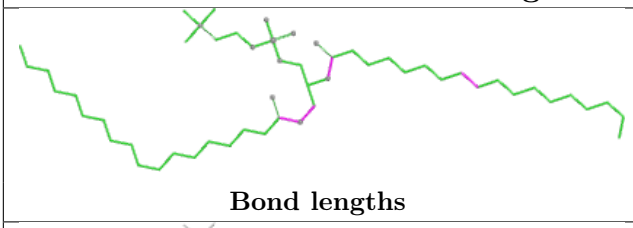


Rings

Ligand OPC A 305



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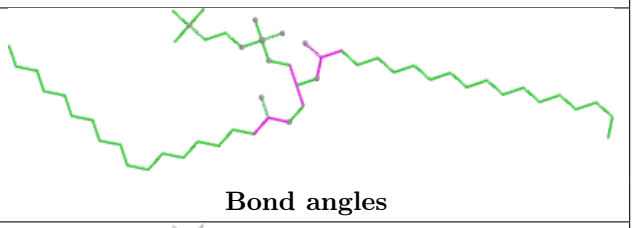
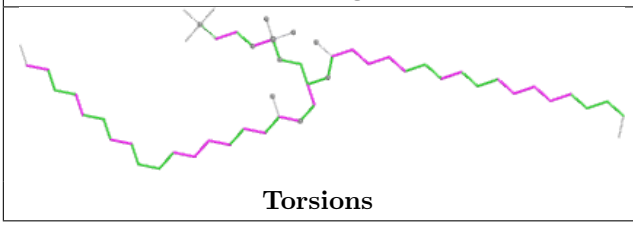
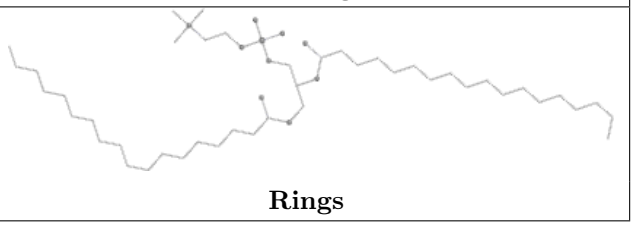


Bond angles

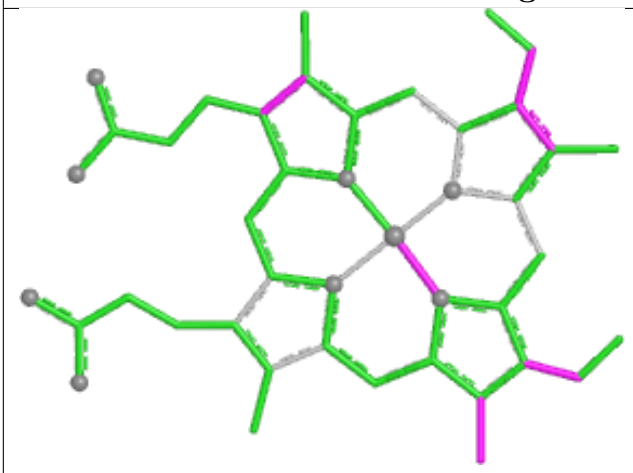


Torsions

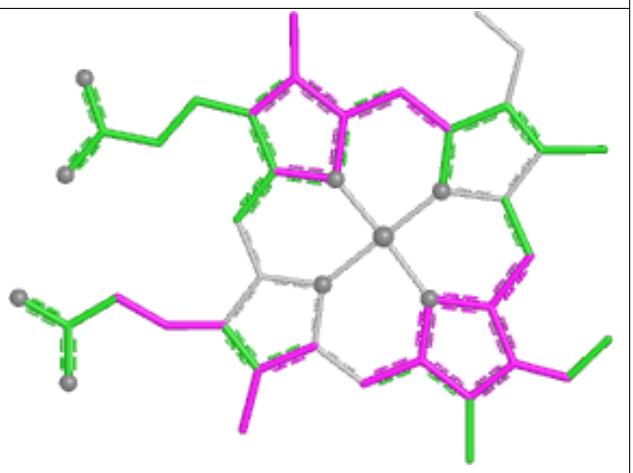


Rings

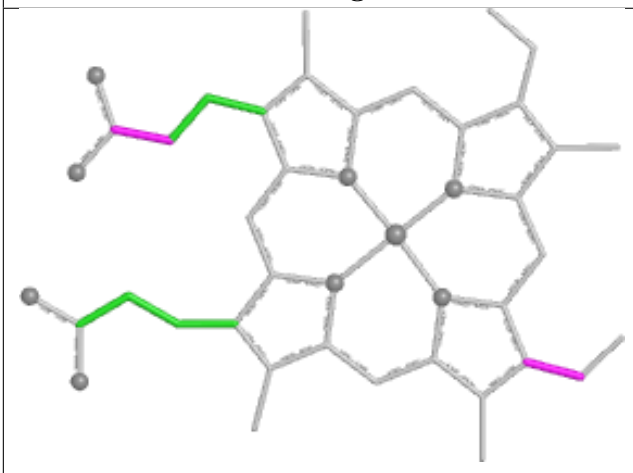
Ligand HEM C 302



Bond lengths



Bond angles



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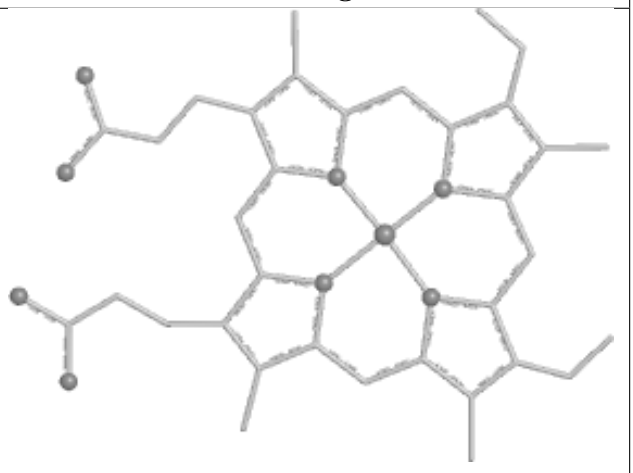
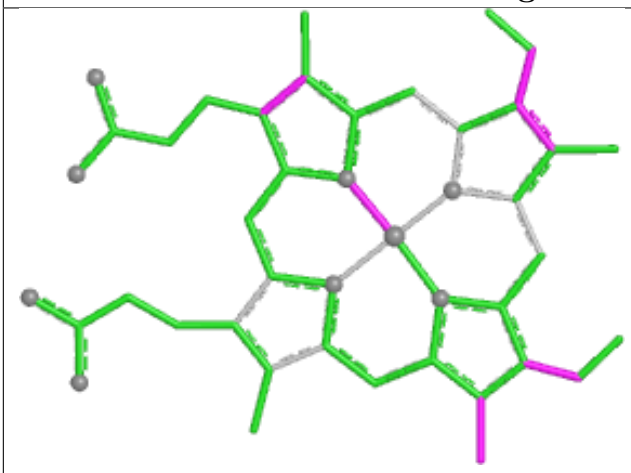
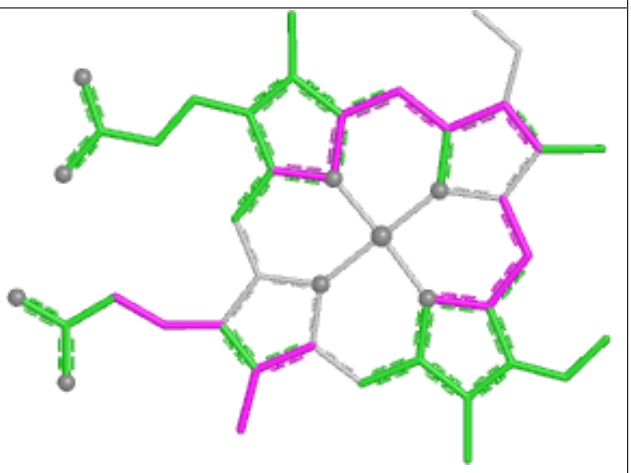


Rings

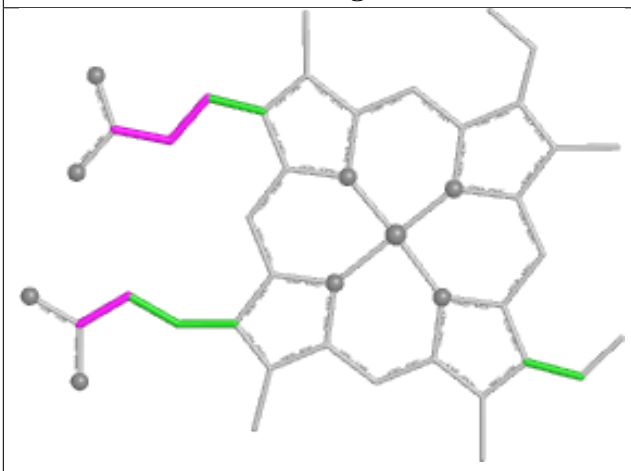
Ligand HEM A 302



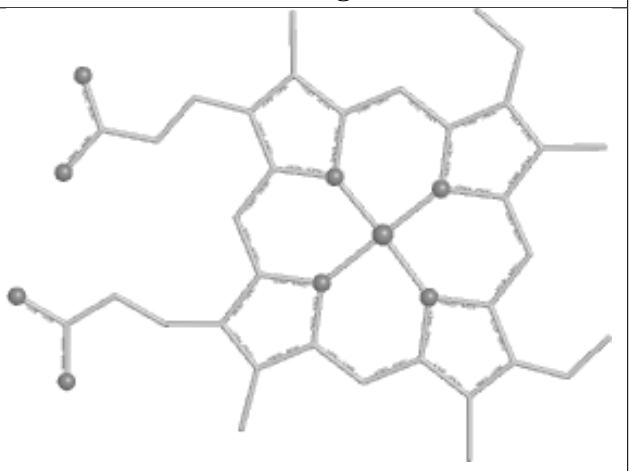
Bond lengths



Bond angles

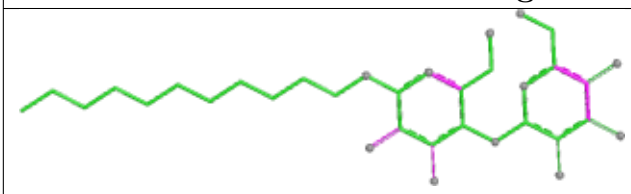


Torsions

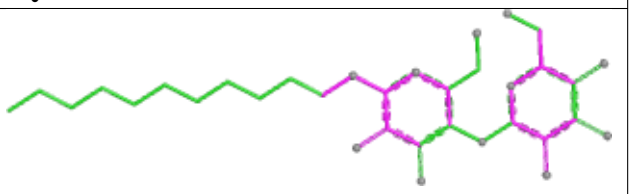


Rings

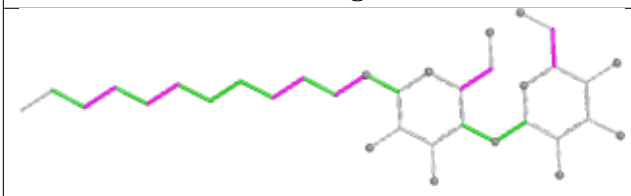
Ligand UMQ A 307



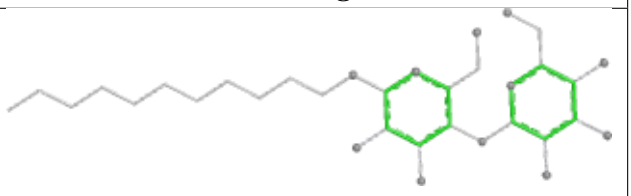
Bond lengths



Bond angles

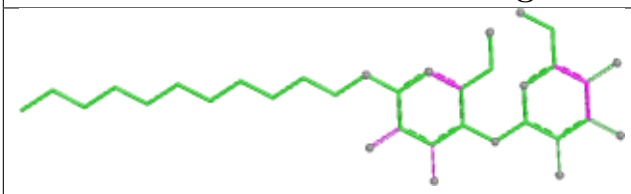


Torsions

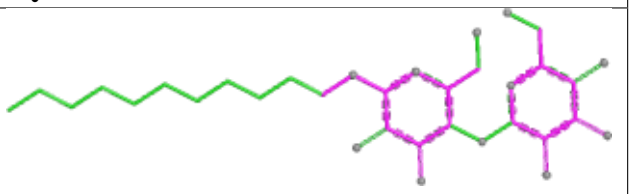


Rings

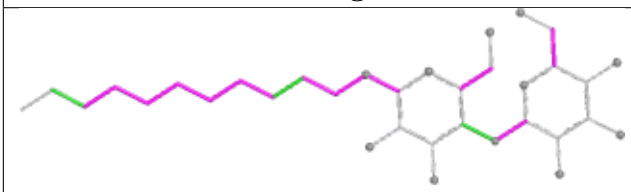
Ligand UMQ A 309



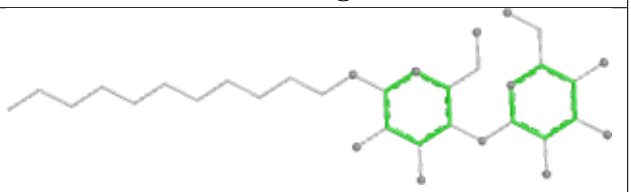
Bond lengths



Bond angles

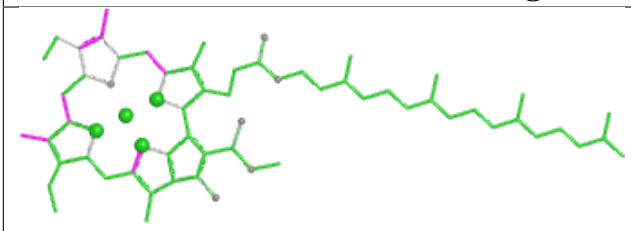


Torsions

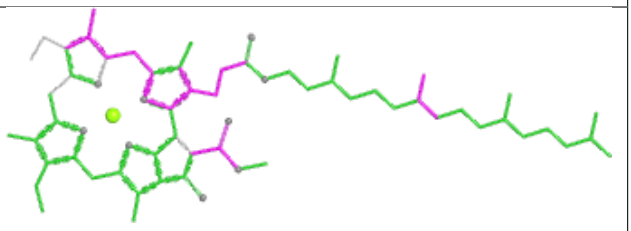


Rings

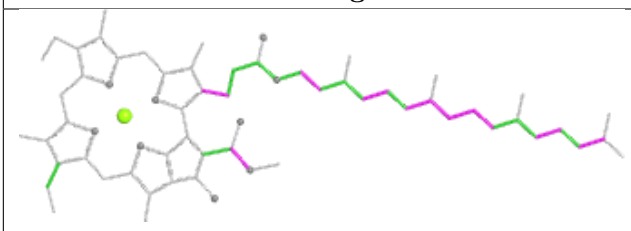
Ligand CLA B 202



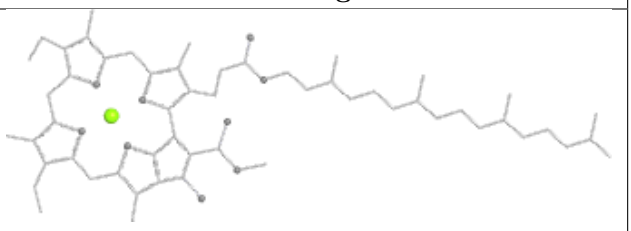
Bond lengths



Bond angles

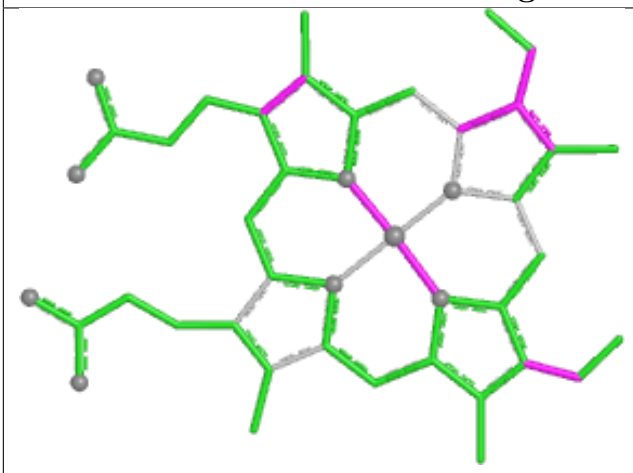


Torsions

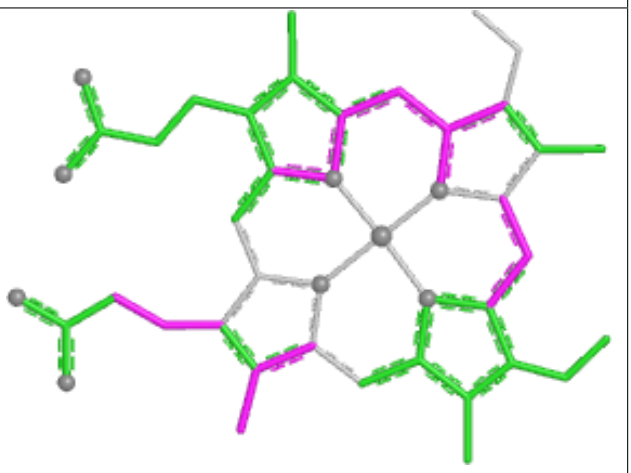


Rings

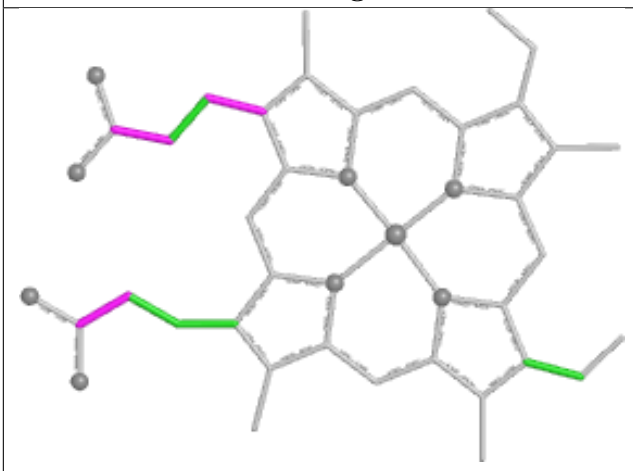
Ligand HEM A 304



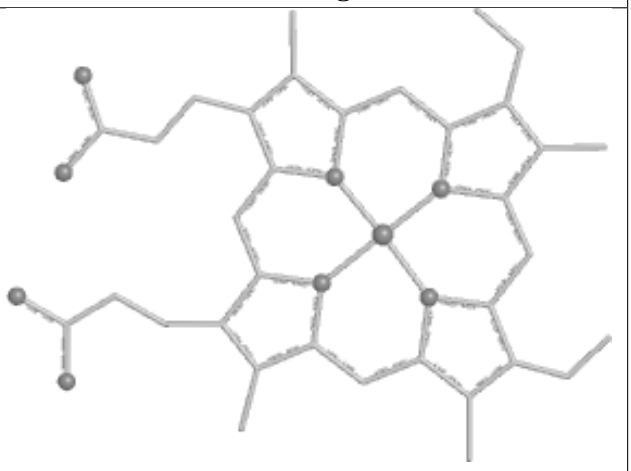
Bond lengths



Bond angles

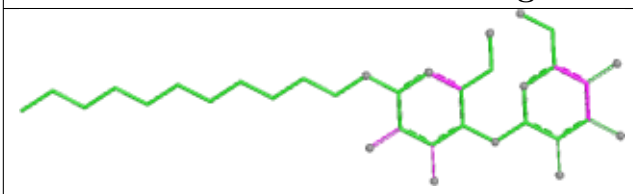


Torsions

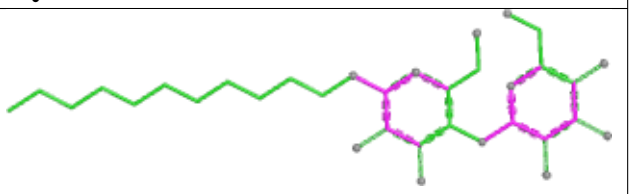


Rings

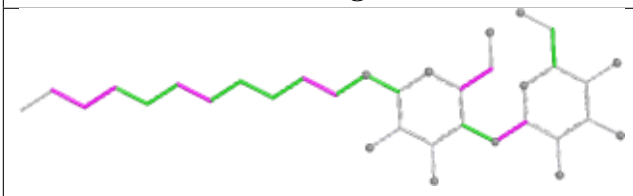
Ligand UMQ C 301



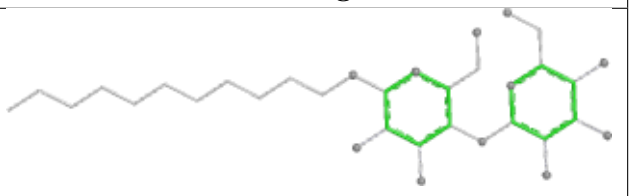
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	213/215 (99%)	0.05	0 100 100	43, 62, 92, 143	0
2	B	160/160 (100%)	0.06	0 100 100	53, 79, 125, 155	0
3	C	286/289 (98%)	0.87	51 (17%) 1 1	57, 91, 188, 215	1 (0%)
4	D	161/179 (89%)	1.68	66 (40%) 0 0	56, 141, 182, 199	0
5	E	32/32 (100%)	0.19	3 (9%) 8 9	72, 94, 125, 148	0
6	F	32/35 (91%)	0.28	1 (3%) 49 47	67, 86, 141, 149	0
7	G	37/37 (100%)	0.24	1 (2%) 54 51	61, 80, 151, 154	0
8	H	29/29 (100%)	0.40	0 100 100	65, 77, 101, 130	0
All	All	950/976 (97%)	0.61	122 (12%) 3 3	43, 84, 174, 215	1 (0%)

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	220	SER	7.9
3	C	199	ILE	6.9
4	D	70	LEU	6.6
3	C	184	ALA	6.6
4	D	160	ILE	6.5

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

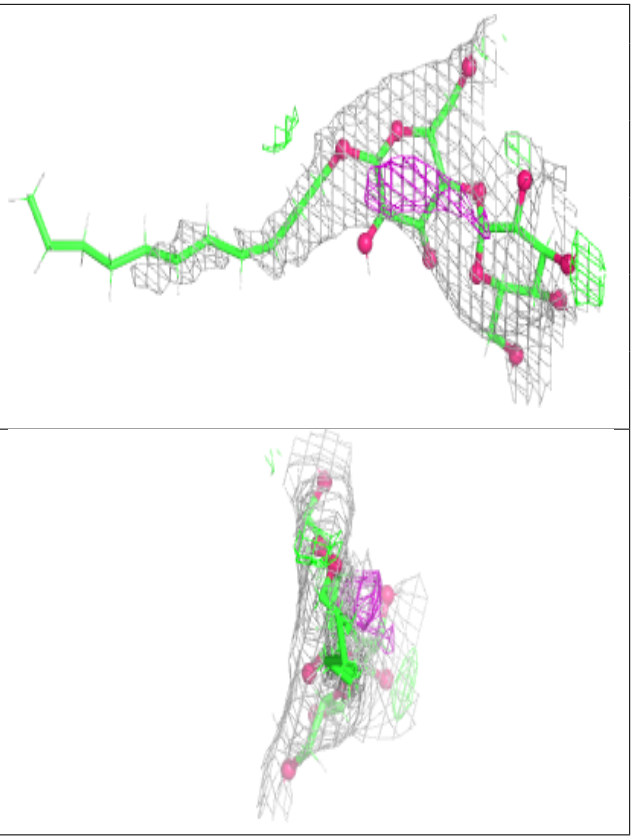
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

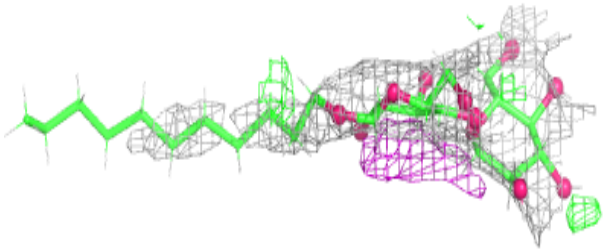
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	UMQ	A	306	34/34	0.71	0.46	61,148,192,198	0
16	SQD	D	201	53/54	0.74	0.55	83,150,191,196	1
12	UMQ	C	301	34/34	0.76	0.52	51,119,203,224	0
12	UMQ	A	309	34/34	0.79	0.33	87,162,229,238	0
11	OPC	A	305	54/55	0.82	0.46	62,118,206,229	0
17	BCR	G	101	40/40	0.82	0.48	51,97,180,199	0
12	UMQ	A	307	34/34	0.86	0.34	81,138,182,186	0
13	QNO	A	308	21/21	0.87	0.34	83,113,154,167	0
11	OPC	B	203	54/55	0.90	0.53	66,126,180,198	0
14	CLA	B	202	65/65	0.95	0.30	59,90,133,153	0
10	HEM	C	302	43/43	0.96	0.29	52,81,118,122	0
15	FES	D	200	4/4	0.96	0.08	108,129,130,138	0
9	CD	B	201	1/1	0.97	0.25	186,186,186,186	0
10	HEM	A	304	43/43	0.97	0.29	54,80,107,112	0
10	HEM	A	303	43/43	0.98	0.29	39,58,82,83	0
9	CD	A	301	1/1	0.98	0.23	83,83,83,83	0
10	HEM	A	302	43/43	0.99	0.29	35,58,79,112	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UMQ A 306:

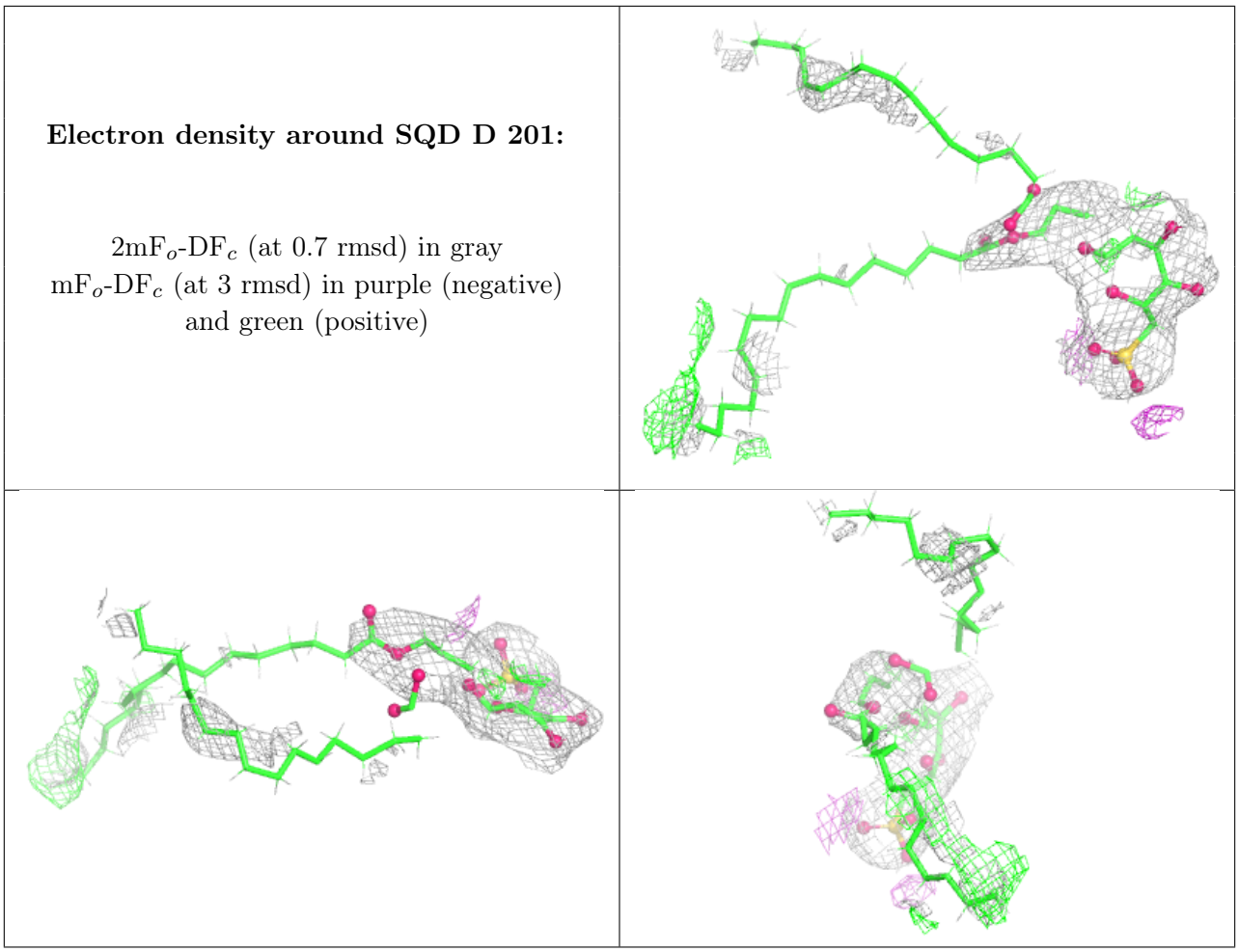
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





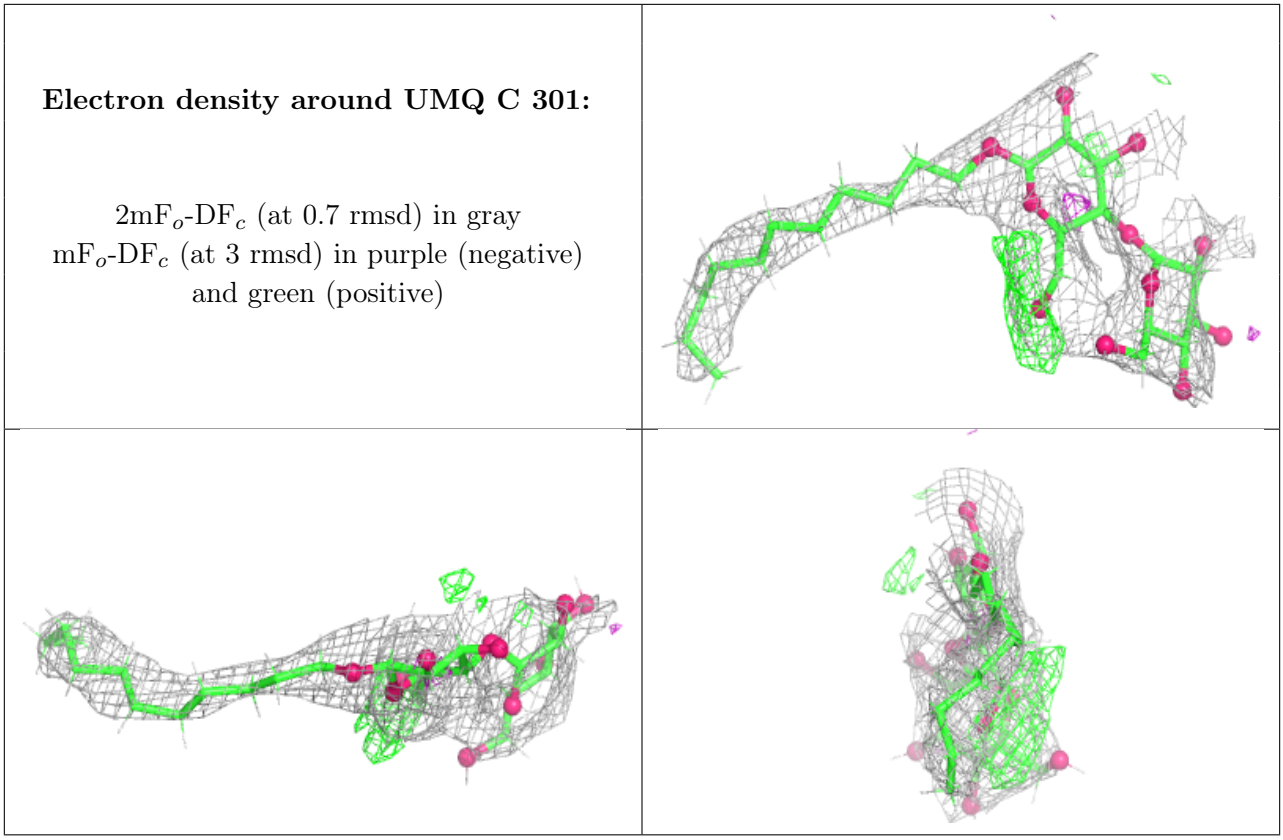
Electron density around SQD D 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



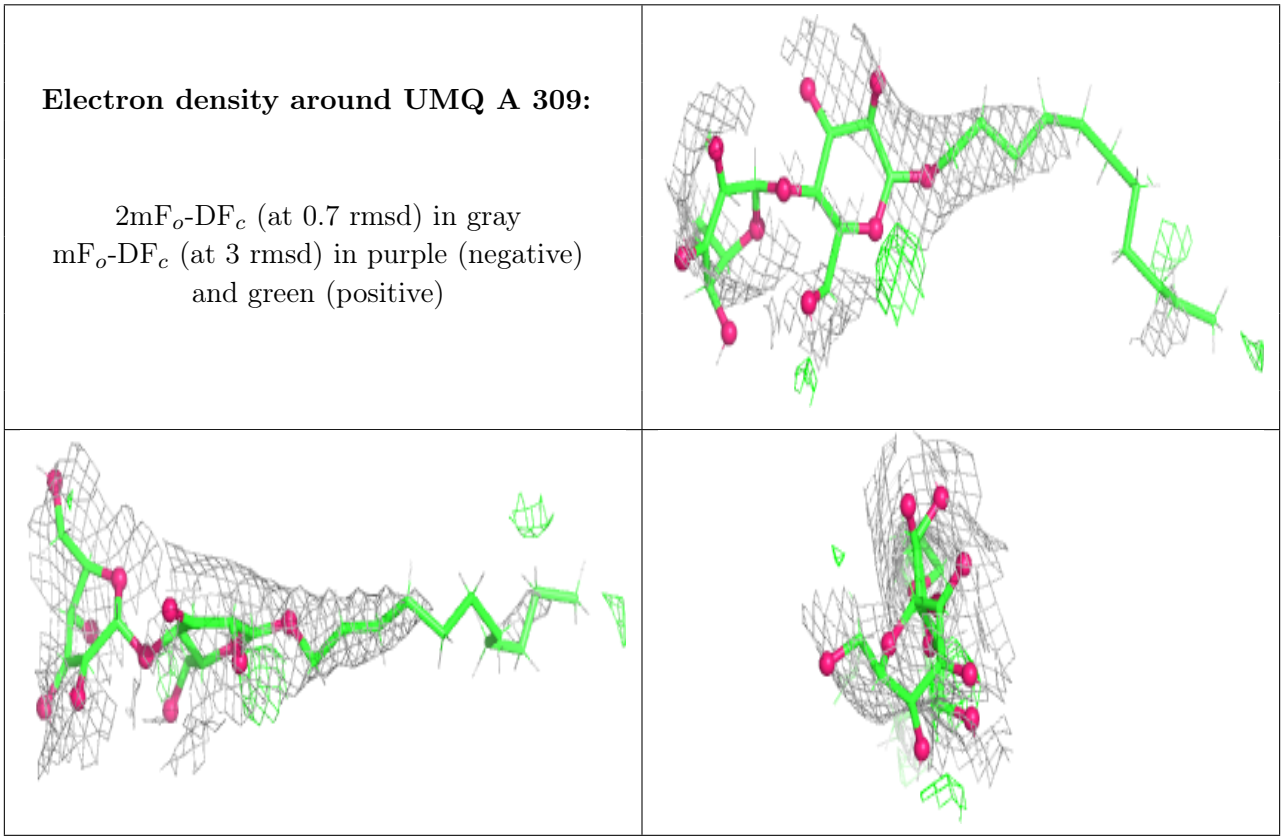
Electron density around UMQ C 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



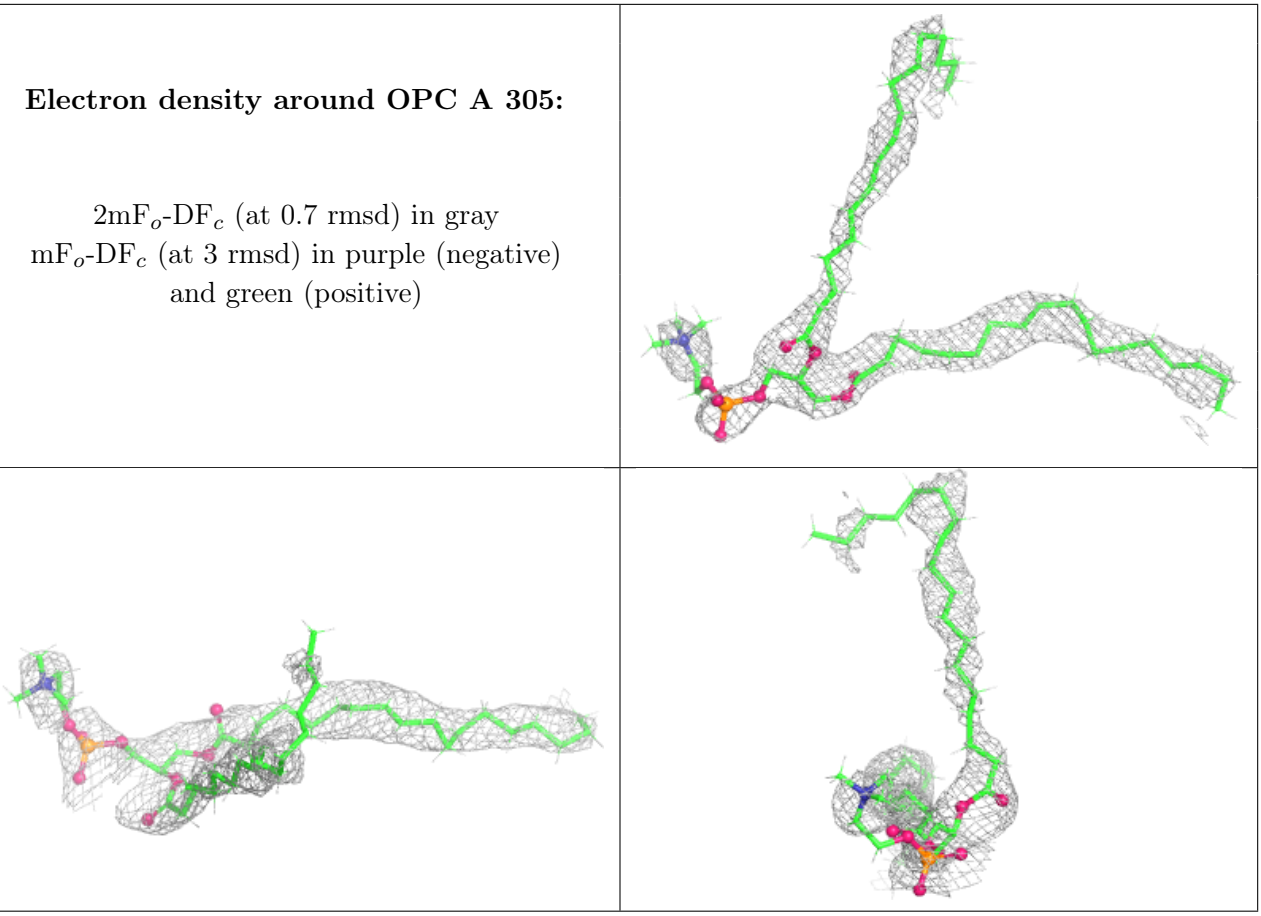
Electron density around UMQ A 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



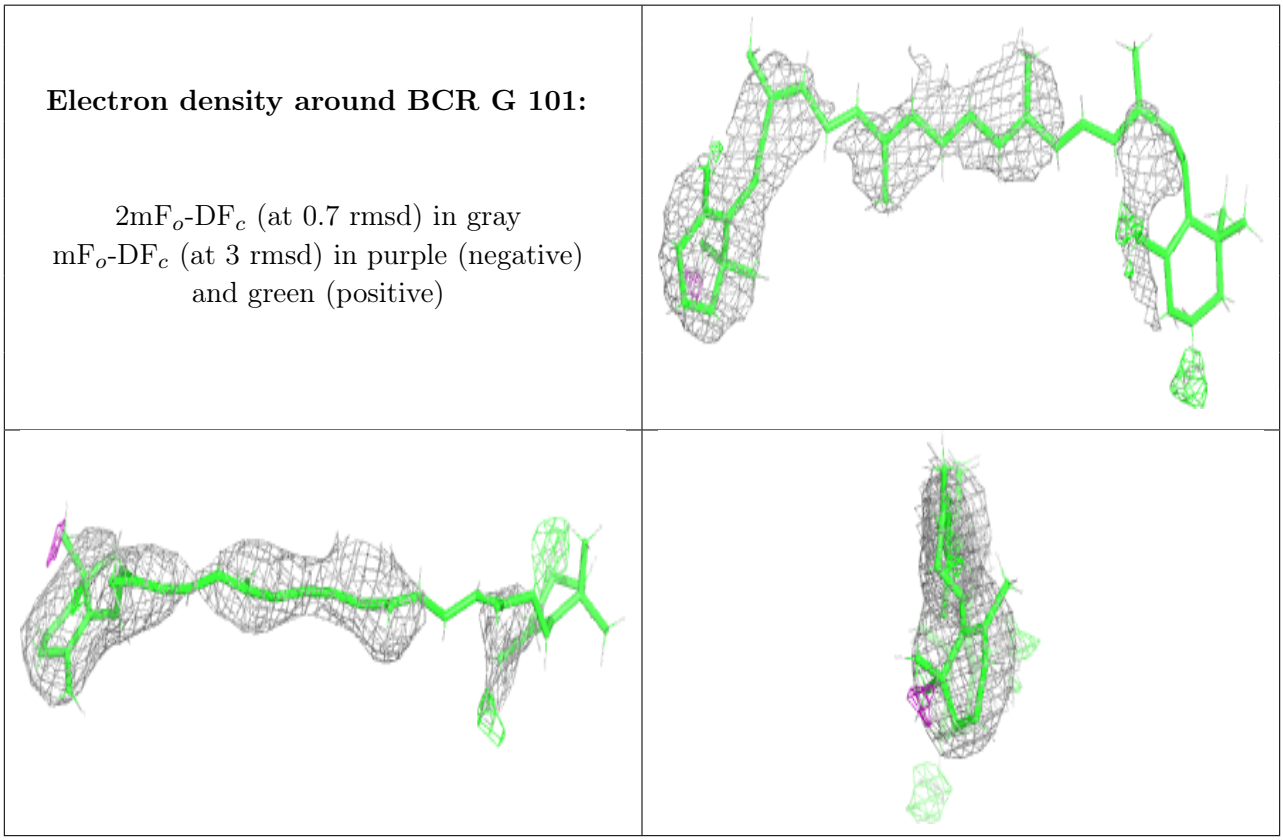
Electron density around OPC A 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



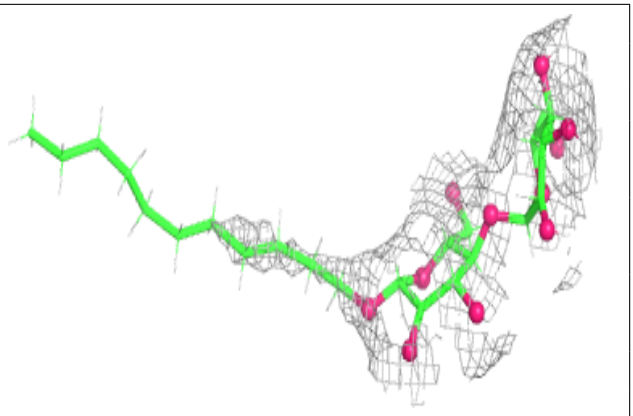
Electron density around BCR G 101:

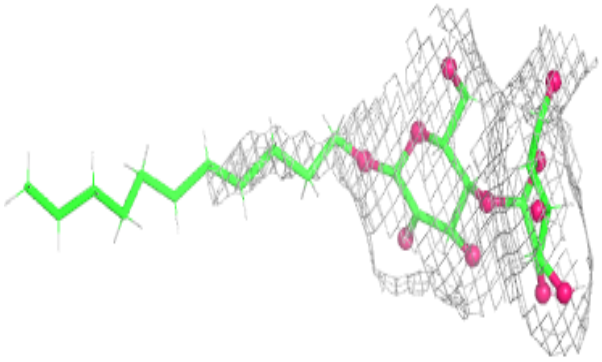
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

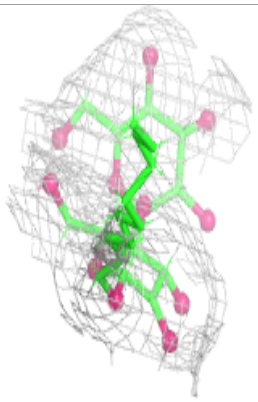


Electron density around UMQ A 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

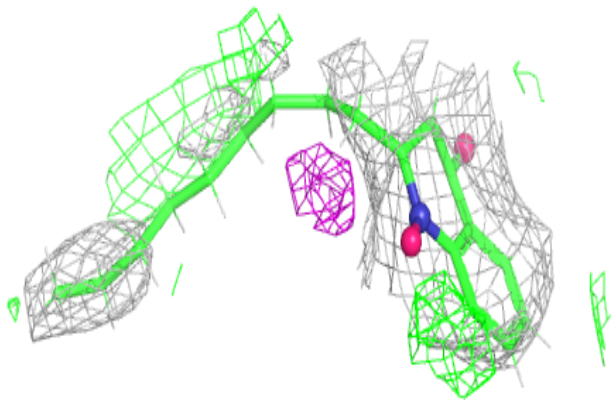


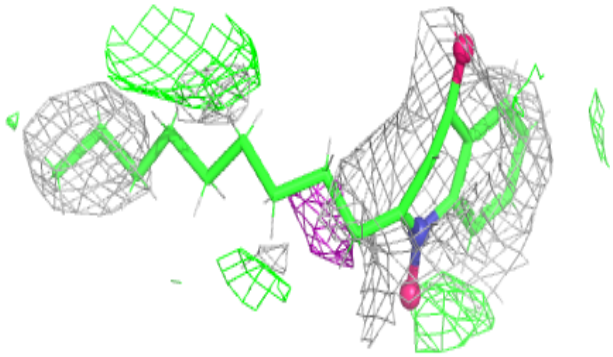


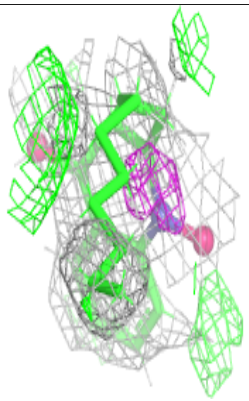


Electron density around QNO A 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

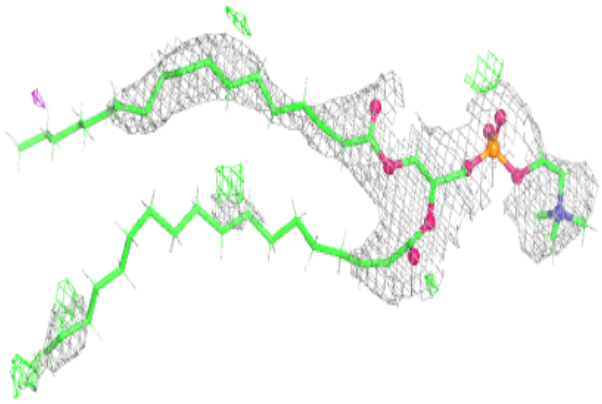


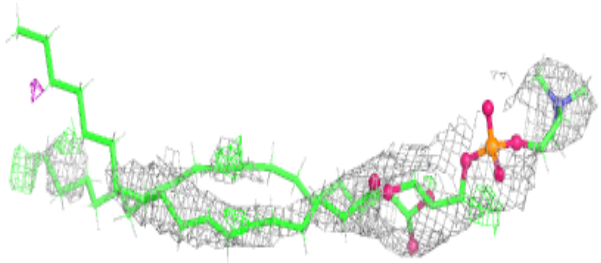




Electron density around OPC B 203:

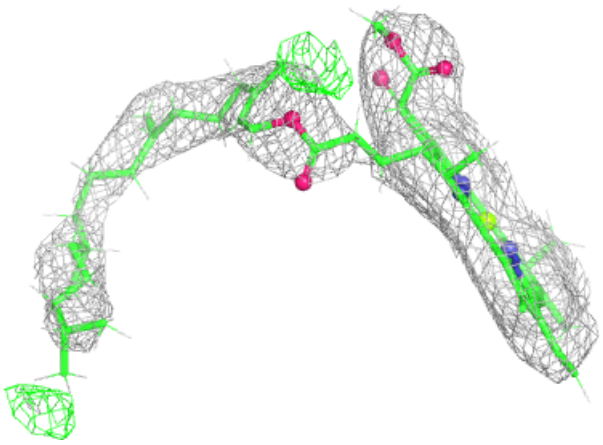
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

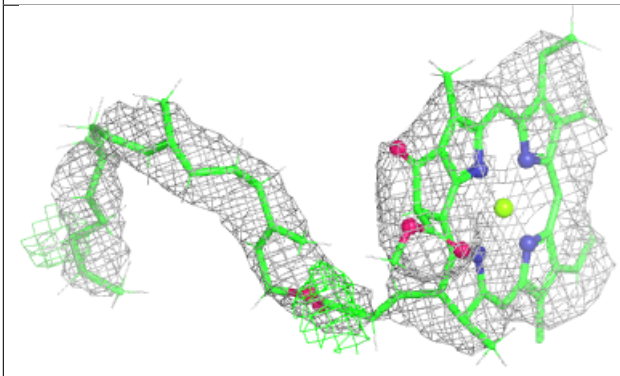


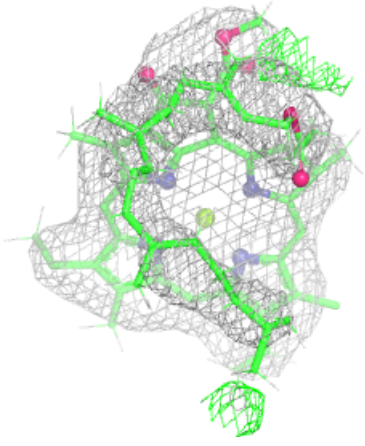


Electron density around CLA B 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

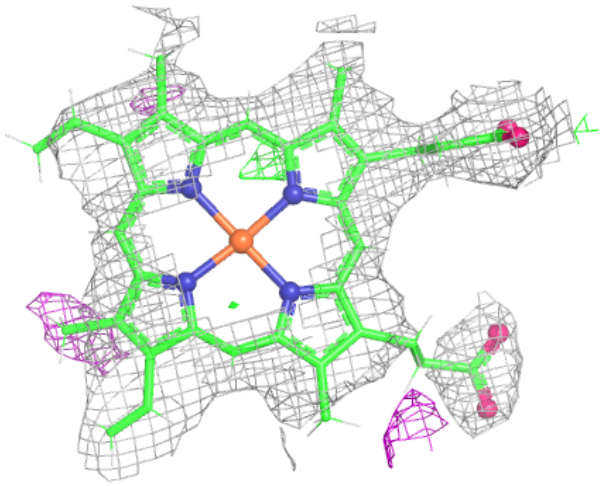


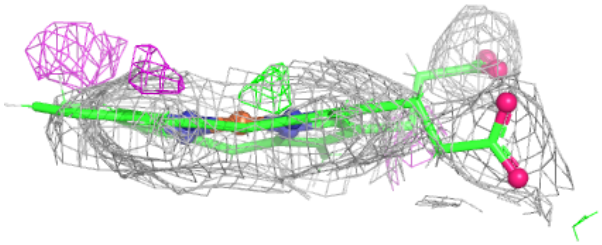


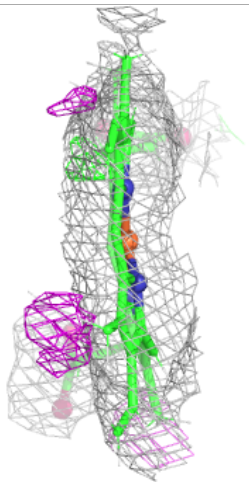


Electron density around HEM C 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

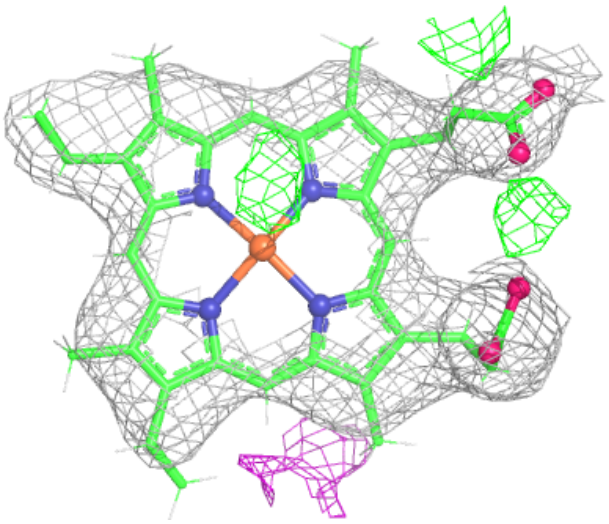


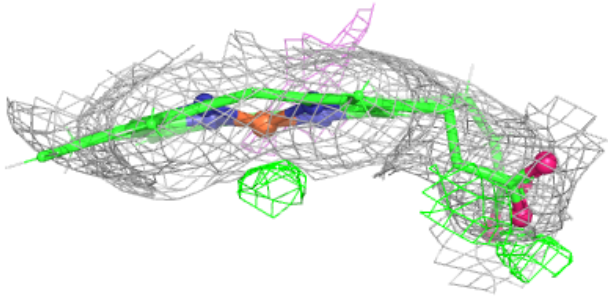


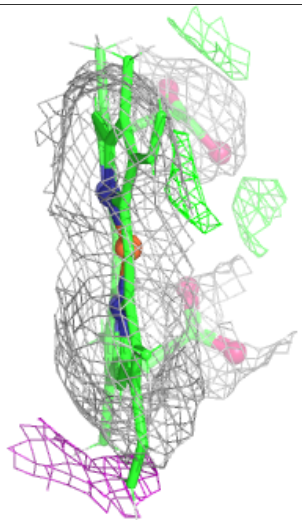


Electron density around HEM A 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

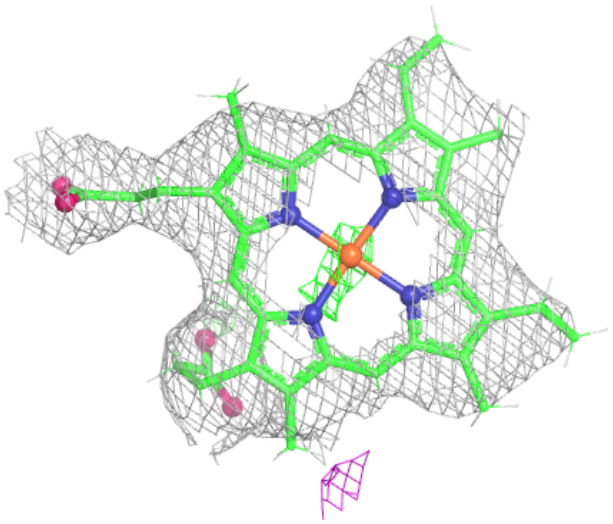


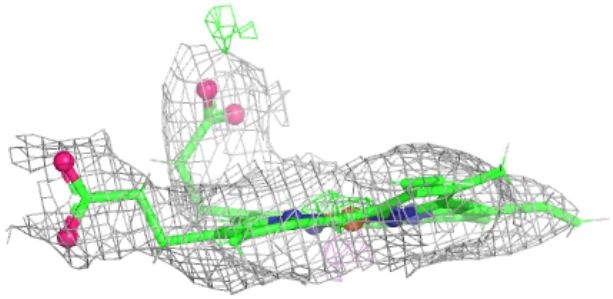


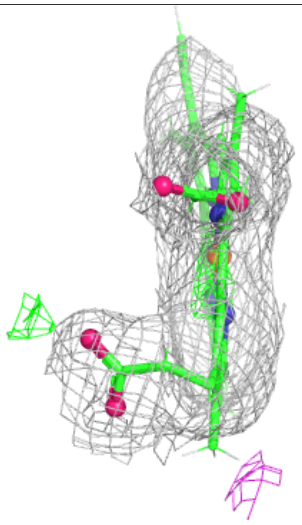


Electron density around HEM A 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

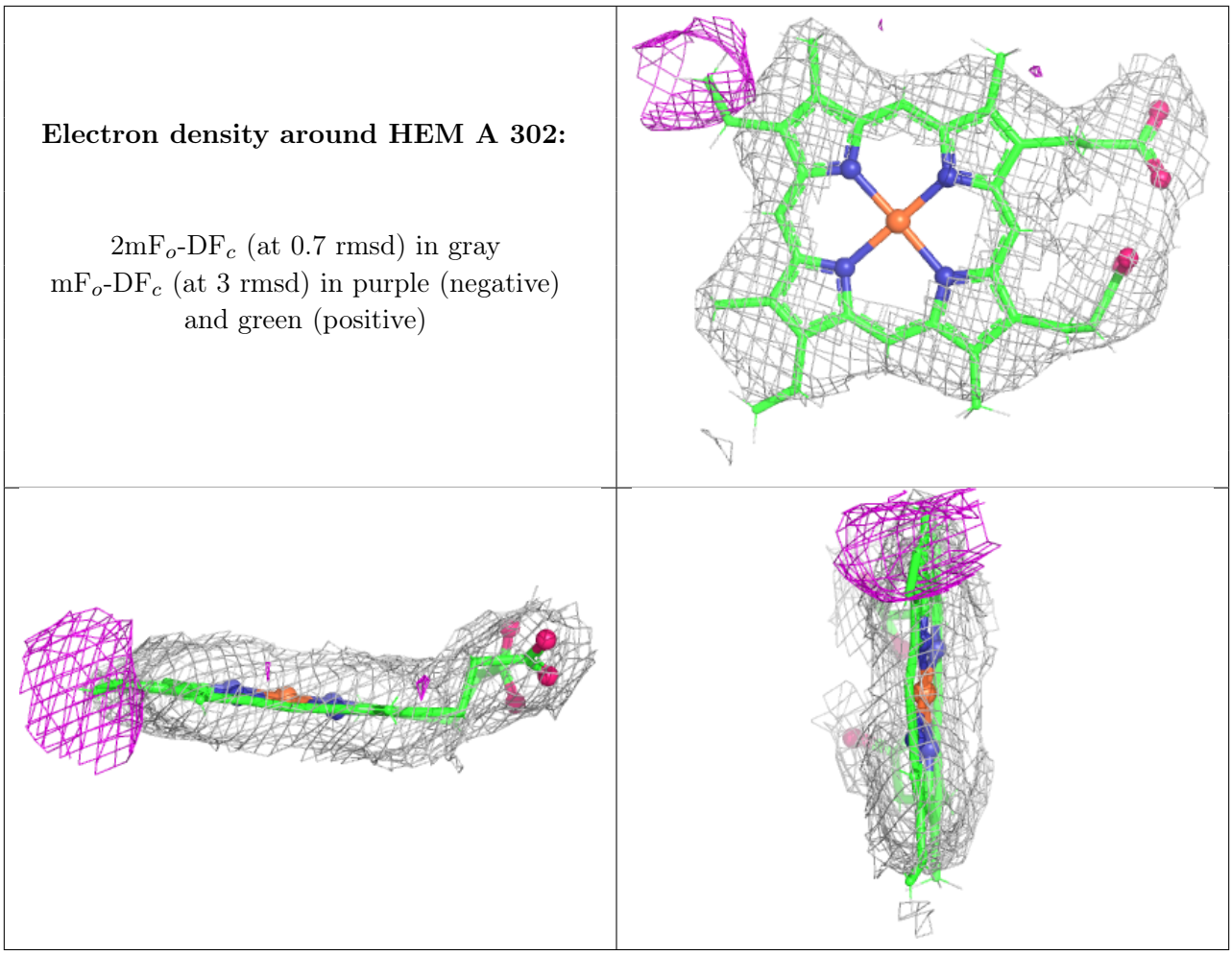






Electron density around HEM A 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.